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* * * * * * * * * Welcome to STN International * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 4	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 5	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 7	AUG 27	USPATOLD now available on STN
NEWS 8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 10	SEP 13	FORIS renamed to SOFIS
NEWS 11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 12	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 13	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS 14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 15	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 16	OCT 19	BEILSTEIN updated with new compounds
NEWS 17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS 18	NOV 19	WPIX enhanced with XML display format
NEWS 19	NOV 30	ICSD reloaded with enhancements
NEWS 20	DEC 04	LINPADOCDB now available on STN
NEWS 21	DEC 14	BEILSTEIN pricing structure to change
NEWS 22	DEC 17	USPATOLD added to additional database clusters
NEWS 23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS 24	DEC 17	DGENE now includes more than 10 million sequences
NEWS 25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 27	DEC 17	CA/CAplus enhanced with new custom IPC display formats
NEWS 28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 29	JAN 02	STN pricing information for 2008 now available
NEWS 30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 31	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 32	JAN 28	MARPAT searching enhanced

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 NEWS 33  JAN 28  USGENE now provides USPTO sequence data within 3 days
                  of publication
 NEWS 34  JAN 28  TOXCENTER enhanced with reloaded MEDLINE segment
 NEWS 35  JAN 28  MEDLINE and LMEDLINE reloaded with enhancements

 NEWS EXPRESS  19 SEPTEMBER 2007:  CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:52:01 ON 01 FEB 2008

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 11:52:06 ON 01 FEB 2008
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STRUCTURE FILE UPDATES:   31 JAN 2008  HIGHEST RN 1001228-41-6
DICTIONARY FILE UPDATES:  31 JAN 2008  HIGHEST RN 1001228-41-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> file casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.46       0.67
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FILE 'CASREACT' ENTERED AT 11:52:10 ON 01 FEB 2008
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FILE CONTENT:1840 - 26 Jan 2008 VOL 148 ISS 5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
************************************************************
*                                                          *
*     CASREACT now has more than 13.8 million reactions    *
*                                                          *
************************************************************
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
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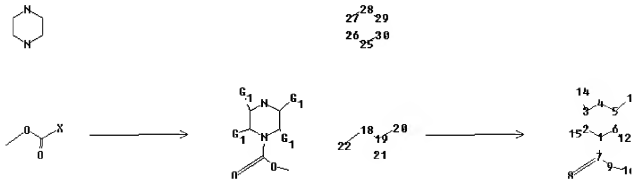

chain nodes :
7 8 9 11 12 14 15 18 19 20 21
ring nodes :
1 2 3 4 5 6 25 26 27 28 29 30
ring/chain nodes :
16 22
chain bonds :
1-7 2-15 3-14 5-11 6-12 7-8 7-9 9-16 18-19 18-22 19-20 19-21

```
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  25-26  25-30  26-27  27-28  28-29  29-30
exact/norm bonds :
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18-22  19-21  25-26  25-30  26-27  27-28  28-29  29-30
exact bonds :
19-20
isolated ring systems :
containing 1 :


G1:C,H,O,X

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  11:CLASS
12:CLASS  14:CLASS  15:CLASS  16:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS
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26:Atom  27:Atom  28:Atom  29:Atom  30:Atom
fragments assigned reactant role:
containing 18
fragments assigned reagent role:
containing 25
fragments assigned product role:
containing 1



L1      STRUCTURE UPLOADED

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L1              STR
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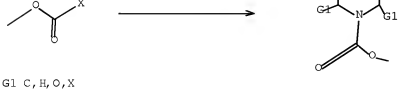

G1 C,H,O,X

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Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
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FULL SEARCH INITIATED 11:52:35 FILE 'CASREACT'
SCREENING COMPLETE - 113 REACTIONS TO VERIFY FROM 11 DOCUMENTS

100.0% DONE 113 VERIFIED 9 HIT RXNS 2 DOCS
SEARCH TIME: 00.00.01

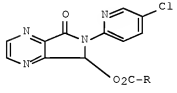
L2 2 SEA SSS FUL L1 (9 REACTIONS)

=> d ibib abs hit

L2 ANSWER 1 OF 2 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 143:211927 CASREACT Full-text
TITLE: Preparation of optically active carbonate intermediates in synthesis of (+)-zopiclone
INVENTOR(S): Bayod Jasanada, Miguel; Sanchez Pedregal, Victor M.; Gotor Santamaria, Vicente; Brieva Collado, M. Rosario; Fernandez Solares, Laura; Diaz Sierra, Monica; Guisan Seijas, Jose Manuel; Paloma Carmona, Jose Miguel; Fernandez-Lafuente, Roberto
PATENT ASSIGNEE(S): Universidad de Oviedo, Spain; Astur Pharma, S.A.
SOURCE: Span., 12 pp.
CODEN: SPXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 2203319	A1	20040401	ES 2002-771	20020403
ES 2203319	B1	20050301		
US 6969767	B1	20051129	US 2003-405998	20030402

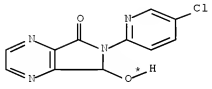
PRIORITY APPLN. INFO.: ES 2002-771 20020403
OTHER SOURCE(S): MARPAT 143:211927
GI



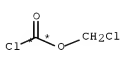
I

AB The invention relates to the synthesis of carbonates I (R = isopropenyloxy, p-nitrophenoxy, chloromethoxy, 1-chloro-, 2-chloro-, 2,2,2-trichloro- or 1,1-dimethyl-2,2,2-trichloroethoxy), their resolution, and use in the synthesis of (+)-zopiclone [(S)-I; R = 4-methyl-1- piperazinyl]. Thus, (S)-I (R = ClCH2O) was prepared by esterification of 6-(5-chloro-2-pyridinyl)-5-hydroxy-7-oxo-5,6-dihydropyrrolo[3,4-b]pyrazine with p-nitrophenyl chloroformate and resolution using immobilized lipase B from Candida antarctica. Treatment of the product with N-methylpiperazine afforded (+)-zopiclone.

RX(14) OF 14 COMPOSED OF RX(7), RX(9), RX(8)
RX(14) A + P + R ===> T



A



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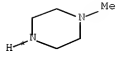
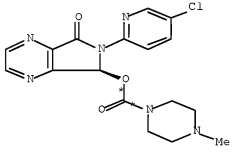


R

3
STEPS



T
YIELD 90%

RX(7) RCT A 43200-81-3, P 22128-62-7
RGT D 110-86-1 Pyridine
PRO Q 508169-18-4
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 17 hours, room temperature

RX(9) RCT Q 508169-18-4
RGT V 290-37-9 Pyrazine
PRO S 508169-20-8
CAT 9001-62-1 Lipase
SOL 7732-18-5 Water, 108-88-3 PhMe
CON 100 hours, 60 deg C, pH 7

```
          NTE  biotransformation, enzymic(immobilized lipase B from Candida
               antarctica used), buffered solution(phosphate), stereoselective

RX(8)     RCT  R 109-01-3, S 508169-20-8
          PRO  T 138729-47-2
          SOL  67-64-1 Me2CO
          CON  SUBSTAGE(1) 0 deg C
               SUBSTAGE(2) 2 hours, 0 deg C -> 15 deg C


=> d l2 ibib abs hit 2


L2   ANSWER 2 OF 2  CASREACT  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         139:307801  CASREACT  Full-text
TITLE:                    Stereoselective alkylation of chiral
                          2-methyl-4-protected piperazines
INVENTOR(S):              Wu, Wenxue; Liao, Hongbiao; Tsai, David J.; Andrews,
                          David R.; Gala, Dinesh; Lee, Gary M.; Schwartz, Martin
                          Lawrence; McAllister, Timothy L.; Fu, Xiaoyong;
                          Maloney, Donal; Thiruvengadam, T. K.; Tann, Chou-Hang
PATENT ASSIGNEE(S):       Schering Corporation, USA
SOURCE:                   PCT Int. Appl., 39 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
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     WO 2003084942     A2    20031016      WO 2003-US9275   20030327
     WO 2003084942     A3    20040506
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU,
             ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD,
             MG, MK, MN, MX, MZ, NI, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG,
             SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2480481        A1    20031016      CA 2003-2480481  20030327
     AU 2003239128     A1    20031020      AU 2003-239128   20030327
     US 2003208074     A1    20031106      US 2003-400429   20030327
     US 6872826        B2    20050329
     EP 1490346        A2    20041229      EP 2003-733842   20030327
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     CN 1642930        A     20050720      CN 2003-807388   20030327
     JP 2005526826     T     20050908      JP 2003-582139   20030327
     CN 101092401      A     20071226      CN 2007-10140725 20030327
     ZA 2004006469     A     20050920      ZA 2004-6469     20040813
     MX 2004PA09414    A     20050125      MX 2004-PA9414   20040928
     US 2005171120     A1    20050804      US 2005-89858    20050325
PRIORITY APPLN. INFO.:                      US 2002-368707P  20020329
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                                            WO 2003-US9275   20030327
OTHER SOURCE(S):          MARPAT 139:307801
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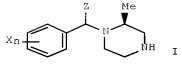
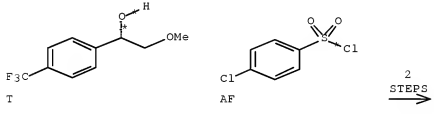
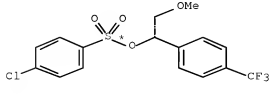


AB Chiral 1-substituted-2-methylpiperazines I [X = alkyl, halogen, haloalkyl, alkoxy, aryl, aryloxy, heteroaryl; n = 1-5; Z = alkyl, alkoxyalkyl, aryl, heteroaryl, heteroaralkyl, aralkyl] are prepared by treating 4-protected (S)-2-methylpiperazine with (S)-XnC6H4CHZO3sY [Y = alkyl, haloalkyl, (un)substituted aryl] and deblocking. Thus, 4-F3CC6H4COCH2OMe was reduced to (S)-4-F3CC6H4CH(OH)CH2OMe with a chiral borane and converted to (S)-4-F3CC6H4CH(CH2OMe)O3SC6H4Cl-4 which was treated with (S)-4-benzyloxycarbpnyl-2-methylpiperazine and deblocked to give I [X = 4-F3C, Z = CH2OMe].

RX(45) OF 104 COMPOSED OF REACTION SEQUENCE RX(10), RX(13)
AND REACTION SEQUENCE RX(2), RX(13)
...T + AF ===> AG...
...A + F + AG ===> AM



T AF



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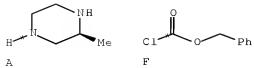
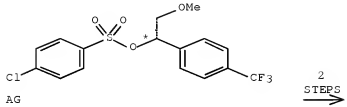
START NEXT REACTION SEQUENCE



A F



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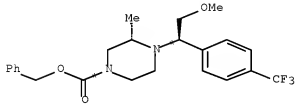

AM
YIELD 85%

RX(10) RCT T 612493-93-3, AF 98-60-2

STAGE(1)
RGT AH 280-57-9 Triethylenediamine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, -5 - -15 deg C
SUBSTAGE(2) 1 hour, -5 - -15 deg C

STAGE(2)
RGT J 7732-18-5 Water

PRO AG 612493-96-6

RX(2) RCT A 74879-18-8, F 501-53-1
RGT H 64-19-7 AcOH
PRO G 612493-87-5
SOL 67-56-1 MeOH, 7732-18-5 Water
CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C
SUBSTAGE(2) 1 hour, 0 - 10 deg C
NTE regioselective

RX(13) RCT G 612493-87-5, AG 612493-96-6
        RGT D 584-08-7 K2CO3
        PRO AM 612494-01-6
        SOL 108-88-3 PhMe, 75-05-8 MeCN
        CON SUBSTAGE(1) room temperature
             SUBSTAGE(2) 30 hours, 80 - 85 deg C
        NTE stereoselective, optimization study

RX(49) OF 104 COMPOSED OF REACTION SEQUENCE RX(10), RX(17)
AND REACTION SEQUENCE RX(5), RX(17)
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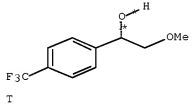
...A + O + AG ===> AK



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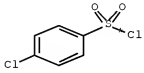
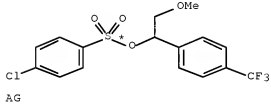


AF

2
STEPS



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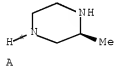
START NEXT REACTION SEQUENCE



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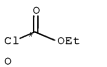

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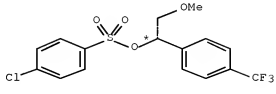

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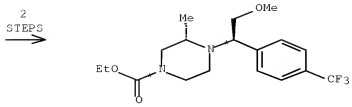

AR
YIELD 88%

RX(10) RCT T 612493-93-3, AF 98-60-2

STAGE(1)
RGT AH 280-57-9 Triethylenediamine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, -5 - -15 deg C
SUBSTAGE(2) 1 hour, -5 - -15 deg C

STAGE(2)
RGT J 7732-18-5 Water

PRO AG 612493-96-6

RX(5) RCT A 74879-18-8, O 541-41-3
RGT H 64-19-7 AcOH
PRO P 612493-91-1
SOL 7732-18-5 Water, 67-56-1 MeOH
CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C
SUBSTAGE(2) 1 hour, 0 - 10 deg C
NTE regioselective

RX(17) RCT P 612493-91-1, AG 612493-96-6
RGT D 584-08-7 K2CO3
PRO AR 612494-06-1
SOL 108-88-3 PhMe, 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 20 hours, 80 - 85 deg C
NTE stereoselective

RX(73) OF 104 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)
AND REACTION SEQUENCE RX(7), RX(10), RX(13)
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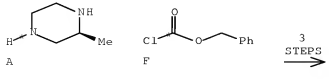
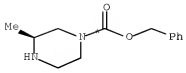
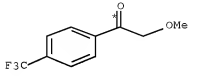
...S + AF + G ===> AM



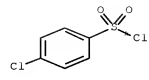


G

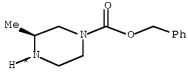
START NEXT REACTION SEQUENCE



S

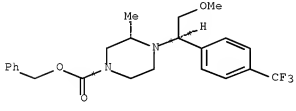


AF



G

3
STEPS



AM
YIELD 85%

RX(2) RCT A 74879-18-8, F 501-53-1
RGT H 64-19-7 AcOH
PRO G 612493-87-5
SOL 67-56-1 MeOH, 7732-18-5 Water
CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C
SUBSTAGE(2) 1 hour, 0 - 10 deg C
NTE regioselective

RX(7) RCT S 26771-69-7

```
            STAGE(1)
               RGT  U 75-75-2 MeSO3H, V 14044-65-6 BH3-THF
               SOL  109-99-9 THF, 108-88-3 PhMe
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 10 minutes, room temperature

            STAGE(2)
               RGT  W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,
                    tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 30 minutes, room temperature

            STAGE(3)
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) 1 hour, 20 - 30 deg C
                    SUBSTAGE(2) 1 hour, room temperature

            STAGE(4)
               SOL  67-56-1 MeOH
               CON  10 - 20 deg C

          PRO  T 612493-93-3
          NTE  stereoselective

RX(10)    RCT  T 612493-93-3, AF 98-60-2

            STAGE(1)
               RGT  AH 280-57-9 Triethylenediamine
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) 1 hour, -5 - -15 deg C
                    SUBSTAGE(2) 1 hour, -5 - -15 deg C

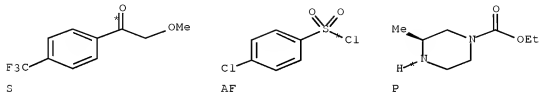
            STAGE(2)
               RGT  J 7732-18-5 Water

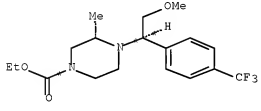
          PRO  AG 612493-96-6

RX(13)    RCT  G 612493-87-5, AG 612493-96-6
          RGT  D 584-08-7 K2CO3
          PRO  AM 612494-01-6
          SOL  108-88-3 PhMe, 75-05-8 MeCN
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) 30 hours, 80 - 85 deg C
          NTE  stereoselective, optimization study


RX(76) OF 104 COMPOSED OF REACTION SEQUENCE RX(5), RX(17)
               AND REACTION SEQUENCE RX(7), RX(10), RX(17)
...A  +  O  ===>  P...
...S  +  AF  +  P  ===>  AP
```

START NEXT REACTION SEQUENCE





AR
YIELD 88%

RX(5) RCT A 74879-18-8, O 541-41-3
RGT H 64-19-7 AcOH
PRO P 612493-91-1
SOL 7732-18-5 Water, 67-56-1 MeOH
CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C
SUBSTAGE(2) 1 hour, 0 - 10 deg C
NTE regioselective

RX(7) RCT S 26771-69-7

STAGE(1)
RGT U 75-75-2 MeSO3H, V 14044-65-6 BH3-THF
SOL 109-99-9 THF, 108-88-3 PhMe

```
            CON  SUBSTAGE(1) room temperature
                 SUBSTAGE(2) 10 minutes, room temperature

         STAGE(2)
            RGT  W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,
                 tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-
            SOL  108-88-3 PhMe
            CON  SUBSTAGE(1) room temperature
                 SUBSTAGE(2) 30 minutes, room temperature

         STAGE(3)
            SOL  108-88-3 PhMe
            CON  SUBSTAGE(1) 1 hour, 20 - 30 deg C
                 SUBSTAGE(2) 1 hour, room temperature

         STAGE(4)
            SOL  67-56-1 MeOH
            CON  10 - 20 deg C

      PRO  T 612493-93-3
      NTE  stereoselective

RX(10)   RCT  T 612493-93-3, AF 98-60-2

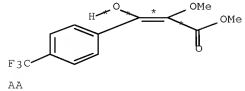
         STAGE(1)
            RGT  AH 280-57-9 Triethylenediamine
            SOL  108-88-3 PhMe
            CON  SUBSTAGE(1) 1 hour, -5 - -15 deg C
                 SUBSTAGE(2) 1 hour, -5 - -15 deg C

         STAGE(2)
            RGT  J 7732-18-5 Water

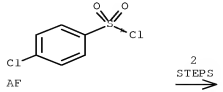
      PRO  AG 612493-96-6

RX(17)   RCT  P 612493-91-1, AG 612493-96-6
      RGT  D 584-08-7 K2CO3
      PRO  AR 612494-06-1
      SOL  108-88-3 PhMe, 75-05-8 MeCN
      CON  SUBSTAGE(1) room temperature
           SUBSTAGE(2) 20 hours, 80 - 85 deg C
      NTE  stereoselective


RX(82) OF 104 COMPOSED OF REACTION SEQUENCE RX(9), RX(7), RX(10), RX(13)
           AND REACTION SEQUENCE RX(2), RX(13)
...AA  +  AF  ===>  AG...
...A  +  F  +  AG  ===>  AM
```

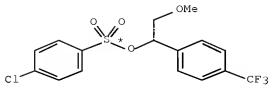


AA



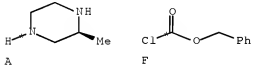
AF

2
STEPS

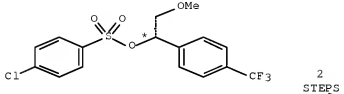


AG

START NEXT REACTION SEQUENCE

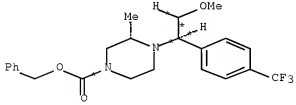


A F



AG

2 STEPS



AM
YIELD 85%

RX(9) RCT AA 612493-95-5
RGT AC 7664-93-9 H2SO4
PRO S 26771-69-7
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) RCT S 26771-69-7

```
            STAGE(1)
               RGT  U 75-75-2 MeSO3H, V 14044-65-6 BH3-THF
               SOL  109-99-9 THF, 108-88-3 PhMe
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 10 minutes, room temperature

            STAGE(2)
               RGT  W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,
                    tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 30 minutes, room temperature

            STAGE(3)
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) 1 hour, 20 - 30 deg C
                    SUBSTAGE(2) 1 hour, room temperature

            STAGE(4)
               SOL  67-56-1 MeOH
               CON  10 - 20 deg C

         PRO  T 612493-93-3
         NTE  stereoselective

RX(10)   RCT  T 612493-93-3, AF 98-60-2

            STAGE(1)
               RGT  AH 280-57-9 Triethylenediamine
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) 1 hour, -5 - -15 deg C
                    SUBSTAGE(2) 1 hour, -5 - -15 deg C

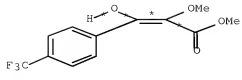
            STAGE(2)
               RGT  J 7732-18-5 Water

         PRO  AG 612493-96-6

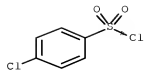
RX(2)    RCT  A 74879-18-8, F 501-53-1
         RGT  H 64-19-7 AcOH
         PRO  G 612493-87-5
         SOL  67-56-1 MeOH, 7732-18-5 Water
         CON  SUBSTAGE(1) 90 minutes, 0 - 10 deg C
              SUBSTAGE(2) 1 hour, 0 - 10 deg C
         NTE  regioselective

RX(13)   RCT  G 612493-87-5, AG 612493-96-6
         RGT  D 584-08-7 K2CO3
         PRO  AM 612494-01-6
         SOL  108-88-3 PhMe, 75-05-8 MeCN
         CON  SUBSTAGE(1) room temperature
              SUBSTAGE(2) 30 hours, 80 - 85 deg C
         NTE  stereoselective, optimization study


RX(87) OF 104 COMPOSED OF REACTION SEQUENCE RX(9), RX(7), RX(10), RX(17)
              AND REACTION SEQUENCE RX(5), RX(17)
...AA  +  AF  ===>  AG...
...A  +  O  +  AG  ===>  AR
```

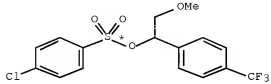


AA



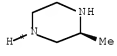
AF

2 STEPS



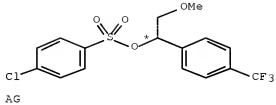
AG

START NEXT REACTION SEQUENCE



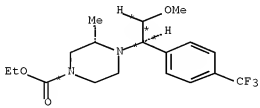
A

O



AG

2 STEPS



AR
YIELD 88%

RX(9) RCT AA 612493-95-5
RGT AC 7664-93-9 H2SO4
PRO S 26771-69-7
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) RCT S 26771-69-7

```
            STAGE(1)
               RGT  U 75-75-2 MeSO3H, V 14044-65-6 BH3-THF
               SOL  109-99-9 THF, 108-88-3 PhMe
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 10 minutes, room temperature

            STAGE(2)
               RGT  W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,
                    tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 30 minutes, room temperature

            STAGE(3)
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) 1 hour, 20 - 30 deg C
                    SUBSTAGE(2) 1 hour, room temperature

            STAGE(4)
               SOL  67-56-1 MeOH
               CON  10 - 20 deg C

         PRO  T 612493-93-3
         NTE  stereoselective

RX(10)   RCT  T 612493-93-3, AF 98-60-2

            STAGE(1)
               RGT  AH 280-57-9 Triethylenediamine
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) 1 hour, -5 - -15 deg C
                    SUBSTAGE(2) 1 hour, -5 - -15 deg C

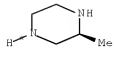
            STAGE(2)
               RGT  J 7732-18-5 Water

         PRO  AG 612493-96-6

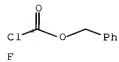
RX(5)    RCT  A 74879-18-8, O 541-41-3
         RGT  H 64-19-7 AcOH
         PRO  P 612493-91-1
         SOL  7732-18-5 Water, 67-56-1 MeOH
         CON  SUBSTAGE(1) 90 minutes, 0 - 10 deg C
              SUBSTAGE(2) 1 hour, 0 - 10 deg C
         NTE  regioselective

RX(17)   RCT  P 612493-91-1, AG 612493-96-6
         RGT  D 584-08-7 K2CO3
         PRO  AR 612494-06-1
         SOL  108-88-3 PhMe, 75-05-8 MeCN
         CON  SUBSTAGE(1) room temperature
              SUBSTAGE(2) 20 hours, 80 - 85 deg C
         NTE  stereoselective


RX(91) OF 104 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)
              AND REACTION SEQUENCE RX(8), RX(9), RX(7), RX(10), RX(13)
...A  +  F  ===>  G...
...Y  +  Z  +  AF  +  G  ===>  AM
```

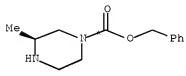


A



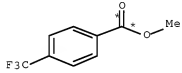
F

5
STEPS

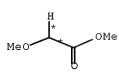


G

START NEXT REACTION SEQUENCE



Y



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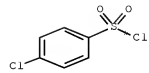
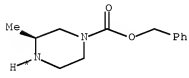
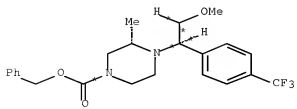


AF



G

5
STEPS



AM
YIELD 85%

```
RX(2)     RCT  A 74879-18-8, F 501-53-1
          RGT  H 64-19-7 AcOH
          PRO  G 612493-87-5
          SOL  67-56-1 MeOH, 7732-18-5 Water
          CON  SUBSTAGE(1) 90 minutes, 0 - 10 deg C
               SUBSTAGE(2) 1 hour, 0 - 10 deg C
          NTE  regioselective

RX(8)     RCT  Y 2967-66-0, Z 6290-49-9

            STAGE(1)
               RGT  AB 124-41-4 NaOMe
               SOL  68-12-2 DMF
               CON  SUBSTAGE(1) 5 hours, -10 deg C
                    SUBSTAGE(2) 21 hours, -10 deg C

            STAGE(2)
               RGT  AC 7664-93-9 H2SO4
               SOL  7732-18-5 Water, 1634-04-4 t-BuOMe
               CON  -8.5 deg C

          PRO  AA 612493-95-5
          NTE  combined yield of 82%

RX(9)     RCT  AA 612493-95-5
          RGT  AC 7664-93-9 H2SO4
          PRO  S 26771-69-7
          SOL  67-56-1 MeOH, 7732-18-5 Water

RX(7)     RCT  S 26771-69-7

            STAGE(1)
               RGT  U 75-75-2 MeSO3H, V 14044-65-6 BH3-THF
               SOL  109-99-9 THF, 108-88-3 PhMe
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 10 minutes, room temperature

            STAGE(2)
               RGT  W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,
                    tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 30 minutes, room temperature

            STAGE(3)
               SOL  108-88-3 PhMe
               CON  SUBSTAGE(1) 1 hour, 20 - 30 deg C
                    SUBSTAGE(2) 1 hour, room temperature

            STAGE(4)
               SOL  67-56-1 MeOH
               CON  10 - 20 deg C

          PRO  T 612493-93-3
          NTE  stereoselective

RX(10)    RCT  T 612493-93-3, AF 98-60-2
```

STAGE(1)
RGT AH 280-57-9 Triethylenediamine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, -5 - -15 deg C
SUBSTAGE(2) 1 hour, -5 - -15 deg C

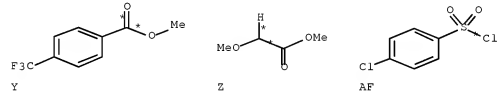
STAGE(2)
RGT J 7732-18-5 Water

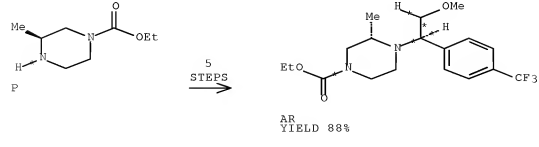
PRO AG 612493-96-6

RX(13) RCT G 612493-87-5, AG 612493-96-6
RGT D 584-08-7 K2CO3
PRO AM 612494-01-6
SOL 108-88-3 PhMe, 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 30 hours, 80 - 85 deg C
NTE stereoselective, optimization study

RX(94) OF 104 COMPOSED OF REACTION SEQUENCE RX(5), RX(17)
AND REACTION SEQUENCE RX(8), RX(9), RX(7), RX(10), RX(17)
...A + Q ===> P...
...Y + Z + AF + P ===> AR

START NEXT REACTION SEQUENCE





RX(5) RCT A 74879-18-8, O 541-41-3
       RGT H 64-19-7 AcOH
       PRO P 612493-91-1
       SOL 7732-18-5 Water, 67-56-1 MeOH
       CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C
            SUBSTAGE(2) 1 hour, 0 - 10 deg C
       NTE regioselective

RX(8) RCT Y 2967-66-0, Z 6290-49-9

         STAGE(1)
            RGT AB 124-41-4 NaOMe
            SOL 68-12-2 DMF
            CON SUBSTAGE(1) 5 hours, -10 deg C
                 SUBSTAGE(2) 21 hours, -10 deg C

         STAGE(2)
            RGT AC 7664-93-9 H2SO4
            SOL 7732-18-5 Water, 1634-04-4 t-BuOMe
            CON -8.5 deg C

       PRO AA 612493-95-5
       NTE combined yield of 82%

RX(9) RCT AA 612493-95-5
       RGT AC 7664-93-9 H2SO4
       PRO S 26771-69-7
       SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) RCT S 26771-69-7

         STAGE(1)
            RGT U 75-75-2 MeSO3H, V 14044-65-6 BH3-THF
            SOL 109-99-9 THF, 108-88-3 PhMe
            CON SUBSTAGE(1) room temperature
                 SUBSTAGE(2) 10 minutes, room temperature

         STAGE(2)
            RGT W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,
                 tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-
            SOL 108-88-3 PhMe
            CON SUBSTAGE(1) room temperature
                 SUBSTAGE(2) 30 minutes, room temperature

         STAGE(3)
            SOL 108-88-3 PhMe
            CON SUBSTAGE(1) 1 hour, 20 - 30 deg C
                 SUBSTAGE(2) 1 hour, room temperature

         STAGE(4)
            SOL 67-56-1 MeOH
            CON 10 - 20 deg C

       PRO T 612493-93-3
       NTE stereoselective

```
RX(10)    RCT  T 612493-93-3, AF 98-60-2

            STAGE(1)
              RGT  AH 280-57-9 Triethylenediamine
              SOL  108-88-3 PhMe
              CON  SUBSTAGE(1) 1 hour, -5 - -15 deg C
                   SUBSTAGE(2) 1 hour, -5 - -15 deg C

            STAGE(2)
              RGT  J 7732-18-5 Water

          PRO  AG 612493-96-6

RX(17)    RCT  P 612493-91-1, AG 612493-96-6
          RGT  D 584-08-7 K2CO3
          PRO  AR 612494-06-1
          SOL  108-88-3 PhMe, 75-05-8 MeCN
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) 20 hours, 80 - 85 deg C
          NTE  stereoselective


=> d his

     (FILE 'HOME' ENTERED AT 11:52:01 ON 01 FEB 2008)

     FILE 'REGISTRY' ENTERED AT 11:52:06 ON 01 FEB 2008

     FILE 'CASREACT' ENTERED AT 11:52:10 ON 01 FEB 2008
L1             STRUCTURE UPLOADED
L2           2 S L1 FULL

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   132.70     133.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -1.50      -1.50

STN INTERNATIONAL LOGOFF AT 11:53:55 ON 01 FEB 2008
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